

## An error analysis of radiance and suboptimal retrieval assimilation

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### SUMMARY

One of the outstanding problems in data assimilation has been, and continues to be, how best to utilize satellite data while balancing the trade-off between accuracy and computational cost. A number of weather-prediction centres have recently achieved remarkable success in improving their forecast skill by changing the method in which satellite data are assimilated into the forecast model from the traditional approach of assimilating retrieved products to the direct assimilation of radiances in a variational framework. Although there are clear theoretical advantages to the direct radiance-assimilation approach, it is not obvious at all to what extent the improvements that have been obtained so far can be attributed to the change in methodology or to various technical aspects of the implementation.

The central question we address here is: how much improvement can we expect from assimilating radiances rather than retrievals, all other things being equal? We compare the two approaches in a simplified theoretical framework. Direct radiance analysis is optimal in this idealized context, while the traditional method of assimilating retrievals is suboptimal because it ignores the cross-covariances between background errors and retrieval errors. We show that interactive retrieval analysis (where the same background used for assimilation is also used in the retrieval step) is equivalent to direct assimilation of radiances with suboptimal analysis weights.

We illustrate and extend these theoretical arguments with several one-dimensional analysis experiments, where we estimate vertical atmospheric profiles using simulated data from temperature sounding channels of both the High-resolution InfraRed Sounder 2 (HIRS2) and the future Atmospheric InfraRed Sounder (AIRS). In the case of non-interactive retrievals the results depend very much on the quality of the background information used for the retrieval step. In all cases, the impact of the choice of analysis method is dwarfed by the effect of changing some of the experimental parameters that control the simulated error characteristics of the data and the retrieval background.

**KEYWORDS:** Data assimilation Radiance Retrievals TIROS (Television Infra-Red Operational Satellite) Operational Vertical Sounder (TOVS)

### 1. INTRODUCTION

A data-assimilation system (DAS) estimates the state of the atmosphere by combining different types of atmospheric observations with a short-term model forecast (often referred to as the first-guess or background field). Assimilated data types include, for example, *in situ* measurements of temperature, moisture, and wind, obtained from radio-sonde soundings. Such conventional observations have a high vertical resolution, but their geographical coverage is mostly limited to land areas in the northern hemisphere. Satellite observations, on the other hand, provide a more uniform spatial coverage but are characterized by a relatively poor vertical resolution. This stems from the fact that the satellite-borne instruments measure quantities that are functions of the atmospheric state variables, such as radiances emitted in certain spectral bands, or integrals of atmospheric refractivity, rather than the state variables themselves.

Two basic approaches have been used to incorporate measurements from remote-sounding instruments, such as the TIROS (Television Infra-Red Operational Satellite) Operational Vertical Sounder (TOVS), in DASs: (1) assimilate radiances (either clear, cloudy, or cloud-cleared to remove the effects of cloud) directly; (2) assimilate geophysical products (retrievals) obtained from the observed radiances. Several operational numerical weather prediction (NWP) centres have recently moved from the more traditional approach of assimilating retrieved products to radiance assimilation using

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variational methods (e.g. Andersson *et al.* 1998; Derber and Wu 1998). There are strong indications that the implementation of direct radiance assimilation at the National Centers for Environmental Prediction (NCEP) has resulted in a large positive impact on forecast skill, both in the northern and southern hemispheres (Derber and Wu 1998). However, a number of changes were introduced simultaneously to the NCEP DAS, including improvements in quality control and systematic error-correction algorithms. It would be extremely interesting to study the performance of various assimilation methods by means of a controlled set of experiments using a fixed DAS and a single, quality-controlled input dataset with a fixed systematic error-correction scheme. However, such a comparison would be difficult to implement. A cleaner comparison was recently conducted at The Met. Office, Bracknell (R. Renshaw, personal communication). These experiments involved assimilating radiances or one-dimensional variational (1D-Var) retrievals using the same radiances and systematic error correction. Radiance assimilation gave a substantially positive impact in the southern hemisphere. The retrieval assimilation was suboptimal in that it assumed the observational errors to be uncorrelated (both vertically and horizontally). However, the observation error covariance was different for the 1D-Var retrievals and the three-dimensional variational (3D-Var) assimilation, with values empirically optimized for both.

The shift toward radiance assimilation has resulted, in part, from theoretical work by Eyre *et al.* (1993), who argued that assimilation of retrieved products amounts to a suboptimal use of the data. Retrievals are produced by combining observations with a prior estimate of the state of the atmosphere, possibly obtained from a forecast model, from climatological data, or from a database of physically feasible vertical profiles. By assimilating the retrievals rather than the radiances into a DAS, additional information from the prior estimate will enter the system along with the measurement information. Errors in retrievals partly depend on the errors in the prior estimate used to produce them, and it is reasonable to expect that the latter are correlated with the errors in the background field used by the DAS, especially in local situations that are important to the DAS. The resulting cross-covariances between retrieval and background errors are not easily quantified and are usually ignored.

In selecting an appropriate assimilation method, computational and other practical issues must be considered as well. Even if radiance assimilation is more desirable from a theoretical point of view, the computational cost of suboptimal retrieval assimilation can be significantly less. This is especially pertinent for advanced sounding instruments such as the Atmospheric InfraRed Sounder (AIRS), which will fly on the National Aeronautics and Space Administration's (NASA) Earth Observing System Post Meridiem (EOS PM) Platform, and the Infrared Atmospheric Sounding Interferometer (IASI), to fly on the European Meteorological Satellite Polar System. These instruments have one or two orders of magnitude more spectral channels available than TOVS. Because of this dramatic increase in data volume, computational costs and simplified logistics may ultimately be the decisive factors in choosing an appropriate assimilation strategy for these instruments. A dedicated science team has been formed for the AIRS instrument whose task, in part, is to produce high-quality retrieved products that could be used for data assimilation. Combining the experience, expertise, and algorithm development of data-assimilation centres and instrument teams would be highly beneficial to both groups. However, when such a team is not present there are other considerations. In the case of data from the National Oceanic and Atmospheric Administration (NOAA)-15 satellite, the raw radiances were available almost a year before operational retrieved products were released. Therefore, users of this radiance data were able to assimilate the data much earlier.

Joiner and da Silva (1998), referred to here as JS, explored various alternatives to radiance assimilation, with an eye toward the assimilation of future data from advanced sounding instruments. For data assimilation systems such as the Physical-space Statistical Analysis System (PSAS) which has been developed at the NASA Goddard Data Assimilation Office (DAO), the computational cost goes up dramatically as the number of observations increases. Computational costs also rise with the number of observations in 3D-Var, although not as dramatically. For AIRS and IASI, the cost of assimilating radiances will be significantly greater than that of assimilating retrievals in the current implementation of the PSAS at the DAO. The number of AIRS radiance measurements for temperature soundings can be 50 times larger than the number of useful pieces of information for a DAS. JS showed that a compact representation of radiances in physical space can be defined which does not retain prior information. The information content of this projection is essentially the same as that of the original set of radiance measurements. Consequently, the assimilation of compressed radiances results in nearly optimal analyses, while retaining some of the practical advantages of traditional retrieval assimilation.

In this paper we address a different question: how much deterioration actually results from a suboptimal analysis of retrieved products due to the reasons stated? Starting from the nonlinear statistical analysis equations, we compare the analysis errors resulting from suboptimal three-dimensional (3D) analysis of one-dimensional (1D) retrievals with the errors that would result from optimal analysis of radiance data. We consider *interactive retrievals*, for which the retrieval prior estimate is identical to the background used in the assimilation system, as a special case. The effect of ignoring the retrieval-background error cross-covariances is illustrated with 1D analysis experiments using simulated data from high- and low-spectral-resolution infrared sounders. Numerical simulations that quantify the additional effect of not properly accounting for horizontal background error correlations will be reported in a follow-up paper.

The outline of the present paper is as follows. In section 2 we review the statistical analysis equations for nonlinear observation operators and derive linearized expressions for the analysis error covariances. This leads to a general error analysis for 3D-Var analysis of radiance data. In section 3 we discuss the production of 1D retrievals and their analysis, and in section 4 we concentrate on interactive retrievals. We are then able to show the precise relation between the two alternatives; in fact, interactive retrieval analysis is linearly equivalent to radiance analysis with a suboptimal gain. We also prove the linear equivalence in a 1D analysis system between optimal radiance analysis and optimal analysis of optimal retrievals. In section 5 we describe the configuration and results of our numerical experiments. We briefly discuss our conclusions and future work in section 6.

## 2. RADIANCE ANALYSIS

The objective of statistical analysis is to produce an accurate estimate of the atmospheric state, given a set of current observations and a background estimate. Satellite-based remote-sounding instruments observe the atmosphere by measuring radiances in a number of spectral intervals for each pixel in the instrument field of view. If the relationship between the radiances and the atmospheric state can be accurately represented by a model, then it is feasible to combine the radiance data directly with the 3D background estimate in a single step.

(a) *The nonlinear analysis equations*

Using the notation defined in JS, the variational framework (e.g. Lorenc 1986; Talagrand 1988) defines the state estimate as the minimum of the functional

$$J(\mathbf{w}) = (\mathbf{w} - \mathbf{w}^f)^T (\mathbf{P}^f)^{-1} (\mathbf{w} - \mathbf{w}^f) + \{\mathbf{w}^o - h(\mathbf{w})\}^T \mathbf{R}^{-1} \{\mathbf{w}^o - h(\mathbf{w})\}, \quad (1)$$

where the unknown vector  $\mathbf{w}$  represents the 3D state of the atmosphere,  $\mathbf{w}^f$  is a background estimate or first guess,  $\mathbf{w}^o$  is a vector of observations,  $\mathbf{P}^f$  is the background error-covariance matrix,  $\mathbf{R}$  is the observation error-covariance matrix, and  $h(\mathbf{w})$  is the observation operator (generally nonlinear) that maps the atmospheric state into observables. In the context of a real-time DAS, the background estimate usually consists of a short-term forecast.

If the background and observations are unbiased, with errors that are normally distributed and uncorrelated with each other, and if the covariances  $\mathbf{P}^f$  and  $\mathbf{R}$  are correctly specified, then the analysis state obtained by minimizing  $J(\mathbf{w})$  is the mode of the conditional probability density function  $p(\mathbf{w} | \mathbf{w}^f \cup \mathbf{w}^o)$ . This renders it optimal in a broad but well defined sense; see Jazwinski (1970).

The minimum of  $J(\mathbf{w})$  can be obtained by a quasi-Newton iteration of the form

$$\mathbf{w}_{i+1} = \mathbf{w}^f + \mathbf{K}_i \{\mathbf{w}^o - h(\mathbf{w}_i) + H_i (\mathbf{w}_i - \mathbf{w}^f)\}, \quad (2)$$

(e.g. Rodgers 1976) where the subscript  $i$  denotes the iteration. A convenient initial iterate is  $\mathbf{w}_0 = \mathbf{w}^f$ , and the matrix  $\mathbf{K}_i$  is the optimal Kalman gain given by

$$\mathbf{K}_i = \mathbf{P}^f H_i^T (H_i \mathbf{P}^f H_i^T + \mathbf{R})^{-1}, \quad (3)$$

and  $H_i$  is a linearized version of  $h$ ,

$$H_i = \left. \frac{\partial h(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}_i}. \quad (4)$$

The analysis vector,  $\mathbf{w}^a$ , is the state obtained at convergence:

$$\mathbf{w}^a = \lim_{i \rightarrow \infty} \mathbf{w}_i. \quad (5)$$

At convergence, Eq. (2) becomes

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K} \{\mathbf{w}^o - h(\mathbf{w}^a) + H(\mathbf{w}^a - \mathbf{w}^f)\} \quad (6)$$

where

$$\mathbf{K} = \mathbf{P}^f H^T (H \mathbf{P}^f H^T + \mathbf{R})^{-1}, \quad (7)$$

$$H = \left. \frac{\partial h(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}=\mathbf{w}^a}. \quad (8)$$

We will refer to Eqs. (6)–(8) as the *nonlinear analysis equations*.

(b) *Linearized analysis error covariances*

If the observation operator is linear, then the matrix,  $H$ , is constant, and  $h(\mathbf{w}^a) = h(\mathbf{w}^f) + H(\mathbf{w}^a - \mathbf{w}^f)$ . Only a single iteration of Eq. (2) is then needed, and the analysis equation (6) simplifies to the familiar form

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K} \{\mathbf{w}^o - h(\mathbf{w}^f)\}. \quad (9)$$

Allowing for possible dependencies among background and observation errors and assuming that  $\mathbf{P}^f$  and  $\mathbf{R}$  are accurate, the error covariance,  $\mathbf{P}^a$ , of the analysis,  $\mathbf{w}^a$ , is given by

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{KH})\mathbf{P}^f(\mathbf{I} - \mathbf{KH})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T + \mathbf{K}\mathbf{X}(\mathbf{I} - \mathbf{KH})^T + (\mathbf{I} - \mathbf{KH})\mathbf{X}^T\mathbf{K}^T, \quad (10)$$

with  $\mathbf{X}$  the background-observation error cross-covariance matrix, and  $\mathbf{I}$  the identity matrix. This expression is valid for any gain matrix  $\mathbf{K}$ , (e.g. for the optimal gain given by Eq. (7) or any suboptimal gain). If background and observation errors are uncorrelated, then  $\mathbf{X} = \mathbf{0}$  and Eq. (10) reduces to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{KH})\mathbf{P}^f(\mathbf{I} - \mathbf{KH})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T. \quad (11)$$

If, in addition,  $\mathbf{K}$  is given by Eq. (7), then this expression further reduces to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{KH})\mathbf{P}^f. \quad (12)$$

In the general case when the observation operator is nonlinear the expressions (10)–(12) can be used to approximate the actual analysis error covariances, by evaluating the linearized observation operator  $H$  at  $\mathbf{w} = \mathbf{w}^a$ . The local accuracy of these approximations then depends on the magnitude of the term  $\{h(\mathbf{w}^a) - h(\mathbf{w}^f) - H(\mathbf{w}^a - \mathbf{w}^f)\}$ .

### (c) Analysis of radiances

The observation operator associated with radiance measurements involves an approximate radiative-transfer or empirical model, which we denote by  $f(\mathbf{z}, \mathbf{b})$ . Such a model can be used to simulate radiances given any atmospheric state,  $\mathbf{z}$ . The vector  $\mathbf{b}$  represents state-independent model parameters, which we assume to be known here. The state variables,  $\mathbf{z}$ , of the radiative-transfer model are generally compatible with the state variables,  $\mathbf{w}$ , of the background—in the sense that both vectors are discrete representations of the same geophysical quantities in the same physical domain. Some parameters in the radiative-transfer model are not state variables (e.g. surface quantities such as emissivity, temperatures above the model top, etc.). These may be included in  $\mathbf{b}$ . In addition,  $\mathbf{z}$  and  $\mathbf{w}$  are not necessarily defined at the same locations. The observation operator associated with radiance assimilation is therefore

$$h(\mathbf{w}) = f(\mathbf{z}, \mathbf{b}) = f(\mathcal{J}\mathbf{w}, \mathbf{b}), \quad (13)$$

where  $\mathcal{J}$  is an interpolation operator (assumed linear throughout) that maps forecast model state variables to the state representation of the radiative-transfer model at the observation location. The linearized observation operator,  $H$ , is

$$H = \frac{\partial h}{\partial \mathbf{w}} = \frac{\partial f}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{w}} = \mathbf{F}\mathcal{J}, \quad (14)$$

with  $\mathbf{F}$  the Jacobian of the radiative-transfer model. Applying the optimal nonlinear analysis equations (6)–(8), we obtain

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^{y_0}\{\mathbf{y} - f(\mathbf{z}^a, \mathbf{b}) + \mathbf{F}(\mathbf{z}^a - \mathbf{z}^f)\}, \quad (15)$$

$$\mathbf{K}^{y_0} = \mathbf{P}^f \mathcal{J}^T \mathbf{F}^T (\mathbf{F} \mathcal{J} \mathbf{P}^f \mathcal{J}^T \mathbf{F}^T + \mathbf{R}^y)^{-1}, \quad (16)$$

$$\mathbf{F} = \left. \frac{\partial f}{\partial \mathbf{z}} \right|_{\mathbf{z}=\mathbf{z}^a}, \quad (17)$$

where  $\mathbf{z}^{a,f} = \mathbf{J}\mathbf{w}^{a,f}$ , and  $\mathbf{R}^y$  is the radiance (or equivalent brightness temperature) error covariance associated with the radiance measurements,  $\mathbf{y}$ . The covariance matrix,  $\mathbf{R}^y$ , accounts for both instrument error and radiative-transfer model error, as discussed by JS, Eyre *et al.* (1993), and by Rodgers (1990).

If the assumption holds that the radiance errors are independent of the background errors and if the linearization error  $\{f(\mathbf{z}^a, \mathbf{b}) - f(\mathbf{z}^f, \mathbf{b}) - F(\mathbf{z}^a - \mathbf{z}^f)\}$  is small, then the linear approximation Eq. (12) applies. The analysis error covariance for optimal radiance analysis is then approximately

$$\begin{aligned}\mathbf{P}^a &\approx (\mathbf{I} - \mathbf{K}^{y_0} \mathbf{F} \mathbf{J}) \mathbf{P}^f (\mathbf{I} - \mathbf{K}^{y_0} \mathbf{F} \mathbf{J})^T + \mathbf{K}^{y_0} \mathbf{R}^y (\mathbf{K}^{y_0})^T \\ &= (\mathbf{I} - \mathbf{K}^{y_0} \mathbf{F} \mathbf{J}) \mathbf{P}^f.\end{aligned}\quad (18)$$

Under ideal circumstances, in the absence of bias and when all error covariances are correctly specified, the nonlinear analysis equations (15)–(17) define the optimal 3D analysis of the radiance data. The expression Eq. (18) then gives a lower bound or benchmark for all other analysis methods.

### 3. RETRIEVAL ANALYSIS

The alternative to radiance analysis is to first produce a set of vertical profiles of atmospheric parameters such as temperature or humidity from the data. The retrieved profiles can then be assimilated as if they were conventional *in situ* observations.

#### (a) Production of one-dimensional retrievals

The retrieval process can be regarded as the solution of a simplified, 1D version of the statistical analysis problem described in the previous section. Retrievals can be thought of as a 3D analysis made up of a composite of 1D vertical profiles defined at a set of horizontal locations, e.g. within a satellite swath. Each of the profiles is obtained by solving a 1D analysis problem based on a subset of the radiance data. A prior-state estimate is needed to supplement the data if the observing system does not completely resolve the vertical structure of the profile. The physics of radiative transfer generally make nadir-viewing instruments insensitive to the high-frequency components of the atmosphere's vertical structure. Therefore, retrievals produced from nadir-sounding microwave and infrared instruments such as the TOVS may include significant information from the prior estimate.

We can write the retrieval state,  $\mathbf{z}^f$ , symbolically as

$$\mathbf{z}^f = \mathbf{D}(\mathbf{y}, \mathbf{b}, \mathbf{z}^p), \quad (19)$$

where  $\mathbf{D}$  denotes a 1D, generally nonlinear, estimator, and  $\mathbf{z}^p$  is the prior-state estimate. As before, the vector  $\mathbf{y}$  represents the radiance data, and  $\mathbf{b}$  are the radiative-transfer model parameters.

Errors associated with 1D retrievals defined at different locations are not independent. It can be shown (e.g. JS) that, if  $\mathbf{P}^p$  is the error covariance associated with the prior-state estimate, and

$$\mathbf{D}_y = \left. \frac{\partial \mathbf{D}}{\partial \mathbf{y}} \right|_{\mathbf{z}=\mathbf{z}^f}, \quad (20)$$

then a linear approximation to the retrieval error covariance is

$$\mathbf{R}^z \approx (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{P}^p (\mathbf{I} - \mathbf{D}_y \mathbf{F})^T + \mathbf{D}_y \mathbf{R}^y \mathbf{D}_y^T. \quad (21)$$

Since  $\mathbf{P}^p$  generally involves horizontal as well as vertical correlations, Eq. (21) shows that the errors in retrievals at different locations must be correlated as well. Note the analogy between this expression for the retrieval error covariance,  $\mathbf{R}^z$ , and Eq. (11); see also Eyre (1987) and Rodgers (1990). The linear operator,  $D_y$ , plays the role of the gain matrix, as will become clear in the following paragraphs.

The optimal 1D estimator,  $D$ , minimizes the likelihood functional

$$J(\mathbf{z}) = (\mathbf{z} - \mathbf{z}^p)^T (\mathbf{P}_{1D}^p)^{-1} (\mathbf{z} - \mathbf{z}^p) + \{\mathbf{y} - f(\mathbf{z}, \mathbf{b})\}^T (\mathbf{R}^y)^{-1} \{\mathbf{y} - f(\mathbf{z}, \mathbf{b})\}. \quad (22)$$

The covariance matrix,  $\mathbf{P}_{1D}^p$ , here is obtained from  $\mathbf{P}^p$  by neglecting all horizontal correlations, i.e. setting them to zero. This corresponds to the fact that some information is lost by replacing the full 3D-Var analysis of section 2(c) by a set of decoupled 1D analyses; information from a sounding at a given location is not allowed to influence the analysis at any other location.

The nonlinear analysis equations of section 2(a) imply that, given a prior-state estimate,  $\mathbf{z}^p$ , and radiance data,  $\mathbf{y}$ , the optimal 1D retrieval satisfies

$$\mathbf{z}^r = \mathbf{z}^p + D_y \{\mathbf{y} - f(\mathbf{z}^r, \mathbf{b}) + F(\mathbf{z}^r - \mathbf{z}^p)\}, \quad (23)$$

$$D_y = \mathbf{P}_{1D}^p F^T (F \mathbf{P}_{1D}^p F^T + \mathbf{R}^y)^{-1}, \quad (24)$$

$$F = \left. \frac{\partial f}{\partial \mathbf{z}} \right|_{\mathbf{z}=\mathbf{z}^r}. \quad (25)$$

A linear approximation to the retrieval error covariance,  $\mathbf{R}^z$ , can be obtained by substituting Eq. (24) into Eq. (21). The accuracy of such an approximation depends on the size of the term  $\{f(\mathbf{z}^r, \mathbf{b}) - f(\mathbf{z}^p, \mathbf{b}) - F(\mathbf{z}^r - \mathbf{z}^p)\}$ .

Da Silva *et al.* (1996) provide statistical evidence for the presence of both horizontally correlated and uncorrelated retrieval error components, consistent with the two terms in Eq. (21). They also show how one can estimate the variances of both components, as well as the decorrelation length of the horizontally correlated component, based on the output of a DAS and radiosonde observations.

### (b) Three-dimensional analysis of one-dimensional retrievals

In traditional retrieval analysis the retrievals,  $\mathbf{z}^r$ , are treated as conventional observations. The observation operator then merely involves interpolation:

$$\mathbf{h}(\mathbf{w}) = \mathbf{J}\mathbf{w}. \quad (26)$$

The analysis equation is simply

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^z (\mathbf{z}^r - \mathbf{J}\mathbf{w}^f). \quad (27)$$

It can be shown that the optimal gain,  $\mathbf{K}^{zo}$ , which properly accounts for non-zero retrieval-background error cross-covariances,  $\mathbf{X}$ , is

$$\mathbf{K}^{zo} = (\mathbf{P}^f \mathbf{J}^T - \mathbf{X}^T) (\mathbf{J} \mathbf{P}^f \mathbf{J}^T + \mathbf{R}^z - \mathbf{J} \mathbf{X}^T - \mathbf{X} \mathbf{J}^T)^{-1}. \quad (28)$$

Numerical solution of the analysis equations with this gain is difficult, because the second factor on the right-hand side of Eq. (28) can be nearly singular. Eyre *et al.* (1993) used the approach of Lorenc *et al.* (1986) to control the associated numerical instabilities, by mapping the 1D retrievals into a reduced space and then modifying both the retrievals and their error variances appropriately.

In practice,  $\mathbf{X}$  is usually neglected because it is difficult to estimate anyway (see, however, da Silva *et al.* (1996)). This results in the suboptimal gain

$$\mathbf{K}^{z_{so}} = \mathbf{P}^f \mathbf{J}^T (\mathbf{J} \mathbf{P}^f \mathbf{J}^T + \mathbf{R}^z)^{-1}. \quad (29)$$

Retrieval analysis with a gain matrix of this form has been implemented operationally in a number of DASs (Susskind and Pfaendtner 1989; Goldberg *et al.* 1993). However, it is clearly not justifiable to assume that retrieval errors are independent of the background errors, i.e. that  $\mathbf{X} = 0$ . Correlations between retrieval and background errors would result, for example, if the latter are correlated with errors in the prior estimate,  $\mathbf{z}^p$ , used for the retrieval production.

For later reference we provide a linear approximation for the analysis error covariance, valid for any gain matrix,  $\mathbf{K}^z$ . Substitution of the optimal 1D retrieval equation (23) into the retrieval analysis equation (27) gives

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^z [\mathbf{z}^p - \mathbf{J} \mathbf{w}^f + \mathbf{D}_y \{ \mathbf{y} - \mathbf{f}(\mathbf{z}^f, \mathbf{b}) + \mathbf{F}(\mathbf{z}^f - \mathbf{z}^p) \}]. \quad (30)$$

If  $\mathbf{X}^{pf}$  is the cross-covariance between prior estimation and background errors, then the linear part of Eq. (30) implies

$$\begin{aligned} \mathbf{P}^a \approx & (\mathbf{I} - \mathbf{K}^z \mathbf{J}) \mathbf{P}^f (\mathbf{I} - \mathbf{K}^z \mathbf{J})^T \\ & + (\mathbf{K}^z - \mathbf{K}^z \mathbf{D}_y \mathbf{F}) \mathbf{P}^p (\mathbf{K}^z - \mathbf{K}^z \mathbf{D}_y \mathbf{F})^T \\ & + (\mathbf{K}^z \mathbf{D}_y) \mathbf{R}^y (\mathbf{K}^z \mathbf{D}_y)^T \\ & + (\mathbf{I} - \mathbf{K}^z \mathbf{J}) \mathbf{X}^{pf} (\mathbf{K}^z - \mathbf{K}^z \mathbf{D}_y \mathbf{F})^T \\ & + (\mathbf{K}^z - \mathbf{K}^z \mathbf{D}_y \mathbf{F}) \mathbf{X}^{pf} (\mathbf{I} - \mathbf{K}^z \mathbf{J})^T. \end{aligned} \quad (31)$$

The first three terms involve the error covariances of the background, radiance observations, and the prior estimate for the retrieval, respectively. The last two terms depend on the matrix  $\mathbf{X}^{pf}$ , which is generally unknown.

#### 4. INTERACTIVE RETRIEVAL ANALYSIS

Interactive retrievals use the background estimate produced by the DAS (i.e. a current short-term forecast) as the prior-state estimate in the retrieval process.

##### (a) Production

We now have

$$\mathbf{z}^p = \mathbf{J} \mathbf{w}^f, \quad (32)$$

$$\mathbf{P}^p = \mathbf{J} \mathbf{P}^f \mathbf{J}^T. \quad (33)$$

Substitution into Eqs. (23)–(25) gives

$$\mathbf{z}^r = \mathbf{J} \mathbf{w}^f + \mathbf{D}_y \{ \mathbf{y} - \mathbf{f}(\mathbf{z}^f, \mathbf{b}) + \mathbf{F}(\mathbf{z}^f - \mathbf{z}^f) \}, \quad (34)$$

$$\mathbf{D}_y = \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T (\mathbf{F} \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T + \mathbf{R}^y)^{-1}, \quad (35)$$

$$\mathbf{F} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \right|_{\mathbf{z}=\mathbf{z}^f}, \quad (36)$$

with  $\mathbf{P}_{1D}^f$  defined by replacing the horizontal correlations in  $\mathbf{P}^f$  by zero.

We obtain an expression for the interactive retrieval error covariance,  $\mathbf{R}^z$ , by substituting Eqs. (35) and (33) into Eq. (21). Some rearrangement yields

$$\mathbf{R}^z \approx (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T + (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{J} (\mathbf{P}^f - \mathbf{P}_{1D}^f) \mathbf{J}^T (\mathbf{I} - \mathbf{D}_y \mathbf{F})^T. \quad (37)$$

It follows directly from the linear part of Eq. (34) that the retrieval-background error cross-covariance,  $\mathbf{X}$ , is approximately

$$\mathbf{X} \approx (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{J} \mathbf{P}^f. \quad (38)$$

Comparison of Eqs. (37) and (38) shows that the retrieval-background error cross-covariance is of the same order of magnitude as the covariance of the retrieval error itself. In fact, if  $\mathbf{P}^f - \mathbf{P}_{1D}^f$  is small then

$$\mathbf{R}^z \approx \mathbf{X} \mathbf{J}^T. \quad (39)$$

This underlines the remark made in section 3 that it is not justifiable to assume that retrieval and background errors are independent. It remains to be seen whether the effect on analysis accuracy of ignoring the cross-covariances (i.e. setting  $\mathbf{X} = 0$ ) is significant in view of the many other approximations that are introduced in practice.

### (b) Analysis

We now consider the analysis of interactive retrievals, first with an unspecified gain matrix,  $\mathbf{K}^z$ . Combining Eqs. (34)–(36) with Eq. (27) gives

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^z \mathbf{D}_y \{ \mathbf{y} - \mathbf{f}(\mathbf{z}^f, \mathbf{b}) + \mathbf{F}(\mathbf{z}^f - \mathbf{z}^f) \}, \quad (40)$$

$$\mathbf{D}_y = \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T (\mathbf{F} \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T + \mathbf{R}^y)^{-1}, \quad (41)$$

$$\mathbf{F} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \right|_{\mathbf{z}=\mathbf{z}^f}. \quad (42)$$

A linear approximation for the associated analysis error covariance is

$$\mathbf{P}^a \approx (\mathbf{I} - \mathbf{K}^z \mathbf{D}_y \mathbf{F} \mathbf{J}) \mathbf{P}^f (\mathbf{I} - \mathbf{K}^z \mathbf{D}_y \mathbf{F} \mathbf{J})^T + \mathbf{K}^z \mathbf{D}_y \mathbf{R}^y (\mathbf{K}^z \mathbf{D}_y)^T. \quad (43)$$

Comparison with the nonlinear analysis equations (15)–(17) for radiance analysis shows precisely the sense in which the analysis of interactive retrievals can be regarded as a suboptimal form of radiance analysis.

First, note that  $\mathbf{z}^a$  is replaced by  $\mathbf{z}^f$  in the nonlinear terms of the analysis equations. This discrepancy is due to the fact that the nonlinear retrieval process has been decoupled from the iterations Eq. (2) of the analysis equations, while all equations are solved simultaneously in the variational approach to radiance analysis.

Second, the gain matrix,  $\mathbf{K}^{y_0}$ , for radiance analysis is replaced by  $\mathbf{K}^z \mathbf{D}_y$  for retrieval analysis. This modifies the linear terms of the analysis equation and should, therefore, represent a significant difference between radiance and retrieval analyses.

### (c) Linear comparison with radiance analysis

Let us now assume that the nonlinear component of the radiative-transfer model is small, in the sense that

$$\mathbf{f}(\mathbf{z}, \mathbf{b}) \approx \mathbf{f}(\mathbf{z}^a, \mathbf{b}) + \mathbf{F}(\mathbf{z} - \mathbf{z}^a) \quad (44)$$

for a constant matrix,  $\mathbf{F}$ . This linearity assumption cannot be expected to be uniformly valid (for all possible retrieval states  $\mathbf{z}$ ), but it should be reasonably accurate locally (for

$\mathbf{z}$  near  $\mathbf{z}^a$  at a given location). Applying Eq. (44) at  $\mathbf{z} = \mathbf{z}^r$  and at  $\mathbf{z} = \mathbf{z}^f$ , both the radiance analysis equation (15) and the interactive retrieval analysis equation (40) can be written

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^y \{\mathbf{y} - \mathbf{f}(\mathbf{z}^f, \mathbf{b})\}, \quad (45)$$

but with

$$\mathbf{K}^y = \mathbf{K}^{y_0} = \mathbf{P}^f \mathbf{J}^T \mathbf{F}^T (\mathbf{F} \mathbf{J} \mathbf{P}^f \mathbf{J}^T \mathbf{F}^T + \mathbf{R}^y)^{-1} \quad (46)$$

for (optimal) radiance analysis, and

$$\mathbf{K}^y = \mathbf{K}^{y_{so}} = \mathbf{K}^z \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T (\mathbf{F} \mathbf{J} \mathbf{P}_{1D}^f \mathbf{J}^T \mathbf{F}^T + \mathbf{R}^y)^{-1} \quad (47)$$

for (suboptimal) retrieval analysis. This shows clearly that interactive retrieval analysis is linearly equivalent to radiance analysis with a suboptimal gain.

Comparison of the two gain matrices shows, first of all, the replacement of  $\mathbf{P}^f$  in Eq. (46) by  $\mathbf{P}_{1D}^f$  in Eq. (47). Horizontal background error correlations are not fully accounted for in retrieval analysis, since the retrievals solve 1D rather than 3D analysis problems. This implies suboptimal use of the available radiance data.

Secondly, the gain matrix for retrieval analysis contains an extra factor,  $\mathbf{K}^z \mathbf{J}$ . Consider, for the moment, the optimal retrieval gain given by Eq. (28). Under the linear approximation, and assuming that  $\mathbf{P}^f - \mathbf{P}_{1D}^f$  is small, it follows from Eq. (39) that

$$\mathbf{K}^z = \mathbf{K}^{z_0} \approx (\mathbf{P}^f \mathbf{J}^T - \mathbf{X}^T)(\mathbf{J} \mathbf{P}^f \mathbf{J}^T - \mathbf{J} \mathbf{X}^T)^{-1}. \quad (48)$$

This expression shows that the optimal gain matrix for retrieval analysis would be identical to that for radiance analysis but for: (1) Omission of the horizontal background error correlations, and (2) interpolation effects. Thus, in a 1D analysis system, optimal radiance analysis and optimal analysis of optimal retrievals are linearly equivalent.

As mentioned earlier, however, use of the optimal retrieval gain is impractical for computational reasons. To show this more clearly, we apply Eq. (39) again to obtain the alternative expression

$$\mathbf{K}^{z_0} = (\mathbf{P}^f \mathbf{J}^T - \mathbf{X}^T)(\mathbf{J} \mathbf{P}^f \mathbf{J}^T - \mathbf{R}^z)^{-1}. \quad (49)$$

The second matrix factor on the right-hand side is difficult to invert, unless all its eigenvalues are bounded away from zero. This condition is violated whenever the observing system does not completely resolve the vertical structure of the profile, because in that case there is at least one mode for which the retrieval accuracy is comparable to or worse than the background accuracy.

Of greater practical interest is the following analysis for the suboptimal retrieval gain,  $\mathbf{K}^z = \mathbf{K}^{z_{so}}$ , defined by Eq. (29), which was obtained by neglecting retrieval-background error cross-covariances. We again assume  $\mathbf{P}^f \approx \mathbf{P}_{1D}^f$ , and consider the two extreme cases when (1) the retrievals are completely determined by the radiance observations alone, or (2) the retrievals depend exclusively on the background, which is the prior-state estimate used in the interactive retrieval process. Substituting Eq. (37) into Eq. (29), we obtain

$$\mathbf{K}^{z_{so}} \mathbf{J} = \mathbf{P}^f \mathbf{J}^T \{\mathbf{J} \mathbf{P}^f \mathbf{J}^T + (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{J} \mathbf{P}^f \mathbf{J}^T\}^{-1} \mathbf{J}. \quad (50)$$

Note that  $\mathbf{K}^{z_{so}} \mathbf{J}$  is the matrix factor that modifies the optimal gain for the radiance data; see Eq. (47). The linear part of the interactive retrieval equation (34) can be written

$$\mathbf{z}^r = (\mathbf{I} - \mathbf{D}_y \mathbf{F}) \mathbf{J} \mathbf{w}^f + \mathbf{D}_y \mathbf{y}. \quad (51)$$

If the state is overwhelmingly determined by the radiance observations, then  $D_y F \approx I$ , i.e. the retrieval is almost independent of the prior estimate  $w^f$  (see JS). Equation (50) then shows that in this case the differences between radiance and retrieval analyses are due only to the appearance of the interpolation operator  $J$ ; neglecting interpolations we have  $K^{z_{so}} J \approx I$ . This shows, not unexpectedly, that in this case the effect of ignoring the cross-covariance terms in the retrieval analysis is negligible.

In the other extreme, suppose that the radiance observations contain virtually no information. Then  $D_y F \approx 0$ , and Eq. (50) then implies that, ignoring interpolation effects, the radiance data are assigned only half as much weight as they should be. On the other hand, Eq. (46) implies that the optimal weights for the radiance data are very small to begin with, in this situation. Therefore, the difference between optimal radiance analysis and suboptimal retrieval analysis is negligible in this case as well.

This argument can be applied to each vertical mode of the retrieved state. The impact of ignoring the retrieval-background error cross-covariances in interactive retrieval analysis is more difficult to assess for modes that depend equally on observational and background information. The 1D numerical simulations reported in the next section will shed some light on this matter.

## 5. ONE-DIMENSIONAL SIMULATION RESULTS

We compare the analysis errors for 1D optimal radiance analysis with those for several suboptimal retrieval analyses, using simulated temperature Jacobians for two different infrared sounders: The AIRS and the High-resolution InfraRed Sounder 2 (HIRS2). This type of 1D experiment represents the vertical structure in a 3D analysis at a location where there is one isolated sounding. HIRS2 has flown continuously on polar-orbiting satellites from 1978 to the present as part of TOVS (see Smith *et al.* 1979). HIRS2 has 19 infrared channels, a single-spot ground field-of-view size at nadir of 17.4 km and scans cross-track  $\pm 49.5^\circ$  from nadir. AIRS is an advanced sounder with over 2000 channels that will fly on the NASA EOS PM platform in the year 2000 (Aumann and Pagano 1994). AIRS has similar spatial resolution and coverage to HIRS2, but the spectral resolution is more than an order of magnitude greater.

We focus here on a single aspect of data assimilation for infrared sounders, namely the temperature profile information contained in the radiances. The simulated HIRS2 channel set includes 11 of the 20 channels (channels 1–7 and 13–16). These are affected mainly by  $CO_2$  absorption and are typically used for temperature soundings. The AIRS channel set includes all 550 available channels between 650 and 742  $cm^{-1}$ , between 2160 and 2270  $cm^{-1}$ , and between 2379 and 2407  $cm^{-1}$ . These are the same channel sets used in JS, and we also prescribe the same instrument-specified noise-equivalent temperatures as in JS. Some of the HIRS2 and AIRS channels are affected by water-vapour absorption and/or the surface skin temperature and emissivity, but for simplicity we assume these variables to be known.

As in JS, the Jacobian,  $F$ , for each instrument is computed using a fast radiative-transfer algorithm based on parametrizations similar to the ones described in Susskind *et al.* (1983). The linearized observation operator,  $H$ , is equal to  $F$ , because for these 1D experiments  $J = I$ . Radiance errors for different channels are assumed independent, with variances equal to the sum of the squared channel noise-equivalent temperatures ( $NE\Delta T$ ) plus an additional  $(0.1\text{ K})^2$  to account for forward model errors. It should be noted that apodization, for an instrument such as IASI, would produce correlated radiance errors. For simplicity, we assume clear-sky night-time (i.e. no reflected solar radiation) and nadir-viewing conditions. These simulations are sufficiently realistic to

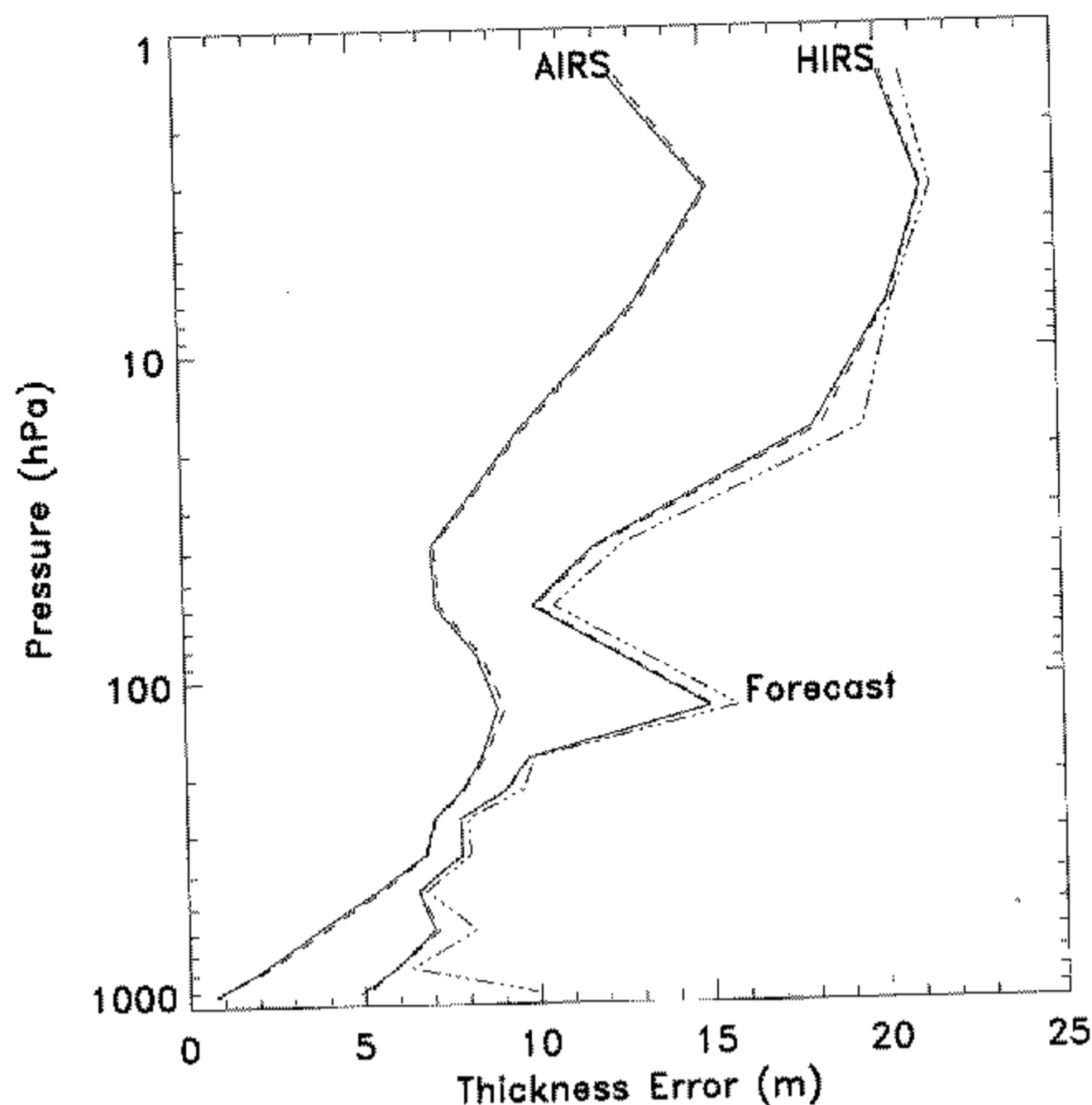


Figure 1. Thickness analysis error standard deviations (m) for optimal radiance assimilation (solid lines) and for interactive retrieval assimilation (dashed lines), using simulated Atmospheric InfraRed Sounder (AIRS) and High-resolution InfraRed Sounder (HIRS) data. Forecast error standard deviations are shown for reference (dot-dashed line).

provide a meaningful comparison between the different analysis methods; in particular, the same simplifying assumptions are made in all cases.

We specify a thickness background error covariance,  $\mathbf{P}^f$ , for our experiments in 17 layers defined between the levels 0.4, 1, 2, 5, 10, 30, 50, 70, 100, 150, 200, 250, 300, 400, 500, 700, 850, and 1000 hPa based on the Goddard EOS DAS 6-hour forecast height error covariances. These were estimated from time series of North American rawinsonde observed-minus-forecast residuals using the method described in Dee and da Silva (1999). Horizontal background error correlations do not play a role in these experiments. Retrieval error covariances originally specified for temperature have been hydrostatically converted to thickness error covariances, while background errors were converted from height to thickness.

For radiance analysis experiments we use the linearized analysis equations (45) and (46), and estimate the analysis errors using Eq. (18). For interactive retrieval analysis we use Eqs. (27) and (29), specify retrieval error covariances according to Eqs. (37) and (35), and estimate the analysis errors using Eq. (43). JS showed by means of Monte Carlo simulations that the linearized expressions for the analysis error covariances approximate the errors for this particular problem quite well, although the actual errors are slightly underestimated.

#### (a) Interactive retrieval analysis

(i) *Using correct retrieval error covariances.* Figure 1 shows the estimated thickness error standard deviations (m), as a function of pressure plotted at the layer mid point, for

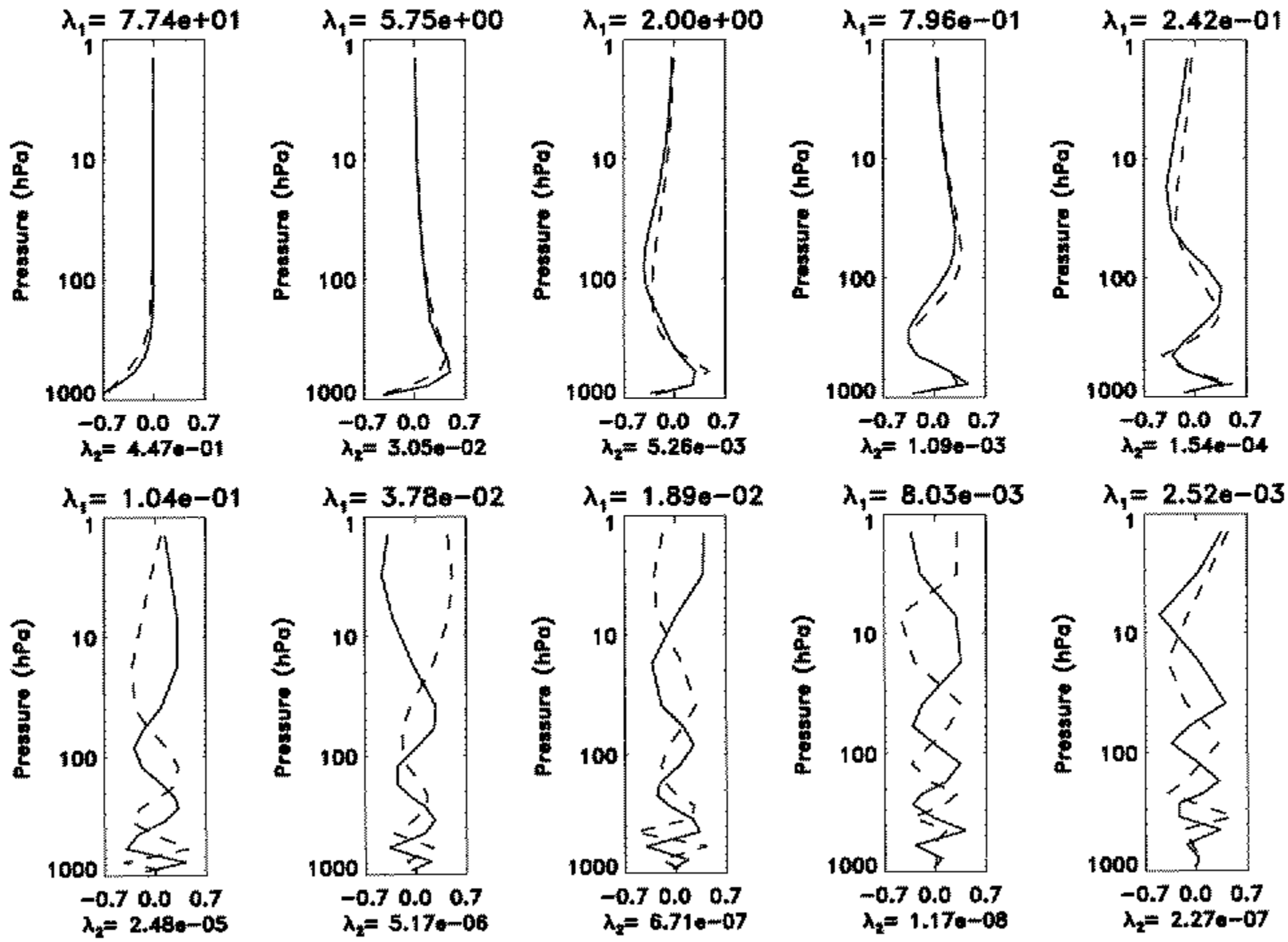


Figure 2. Leading eigenvectors and eigenvalues of  $F^T(\mathbf{R}^y)^{-1}F$  for the Atmospheric InfraRed Sounder (solid line,  $\lambda_1$ ) and the High-resolution InfraRed Sounder (dashed line,  $\lambda_2$ ) for a mid-latitude profile.

radiance analysis (solid curves) and for interactive-retrieval analysis (dashed curves), using either AIRS or HIRS. For reference, the prescribed background-error standard deviations are shown in the figure as well. Since the error covariances are correctly specified for this experiment, interactive-retrieval analysis is suboptimal only because the cross-covariances between retrieval and background errors are not accounted for. The error standard deviations are obtained from the diagonal of the analysis error covariance,  $\mathbf{P}^a$ , computed for each case. The figure shows that the analysis-error standard deviations for the two methods are virtually indistinguishable. Not shown are the thickness analysis-error vertical correlations, which are also nearly identical for the two methods. To gain some insight into this result, we separate the analysis errors into contributions from the background and the radiances.

We project the two components of the analysis error covariance onto the eigenvectors of  $F^T(\mathbf{R}^y)^{-1}F$ , which are the columns of the unitary matrix,  $\mathbf{U}$ , in

$$F^T(\mathbf{R}^y)^{-1}F = \mathbf{U}\mathbf{D}\mathbf{U}^T, \quad (52)$$

with  $\mathbf{D}$  a diagonal matrix of eigenvalues. This transformation was used in JS to produce compact partial eigen-decomposition retrievals. The eigenvectors for the two instruments are shown in Fig. 2 in order of decreasing eigenvalue, that is to say, in order of increasing uncertainty. Accordingly, we can define

$$\mathbf{P}_{(f)}^a = \mathbf{U}^T(\mathbf{I} - \mathbf{K}\mathbf{F})\mathbf{P}^f(\mathbf{I} - \mathbf{K}\mathbf{F})^T\mathbf{U} \quad (53)$$

and

$$\mathbf{P}_{(y)}^a = \mathbf{U}^T\mathbf{K}\mathbf{R}^y\mathbf{K}\mathbf{U}, \quad (54)$$

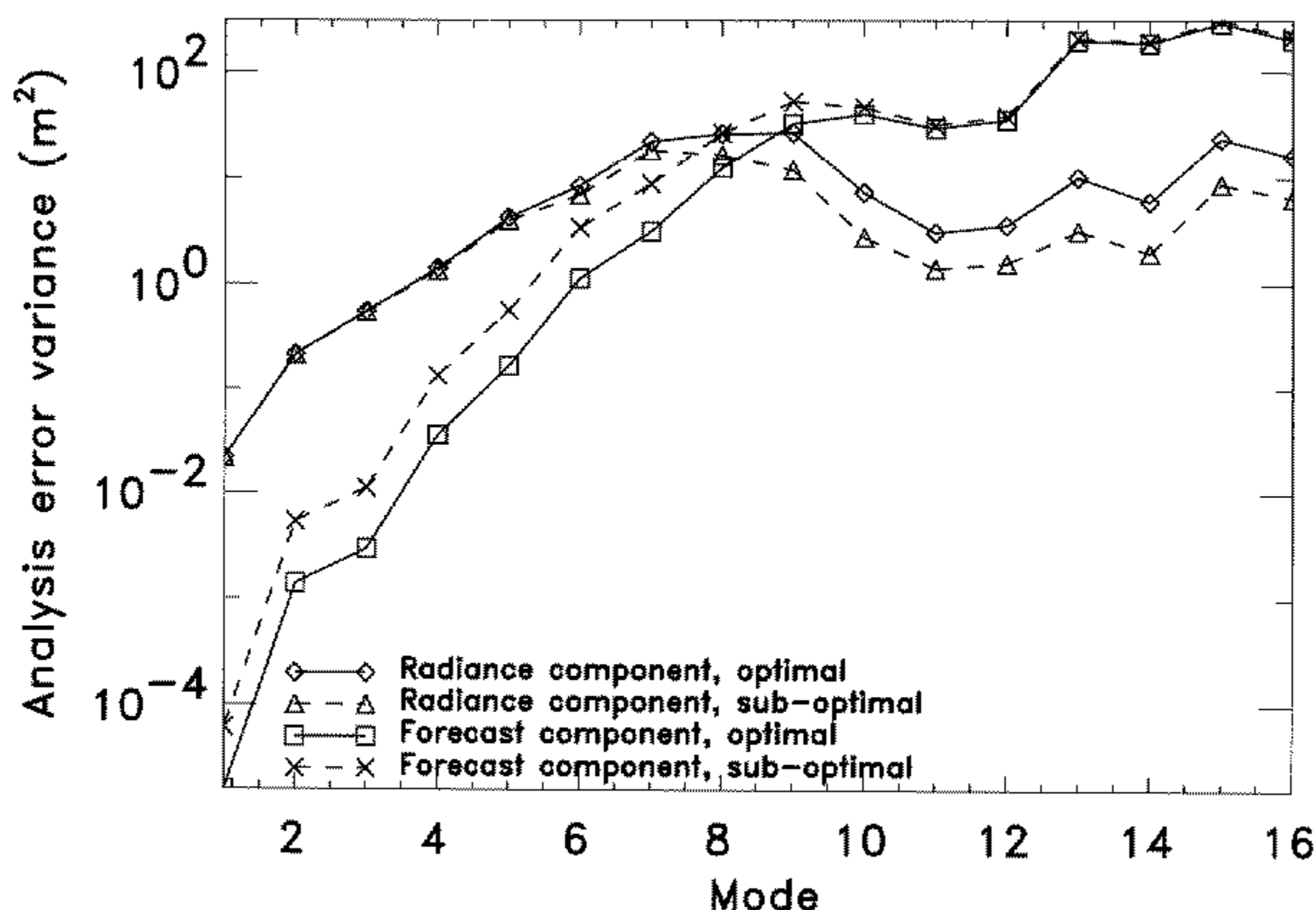


Figure 3. Forecast and radiance contributions to the analysis error variances, projected onto the eigenvectors of Fig. 2, for simulated Atmospheric InfraRed Sounder data.

corresponding to the two terms in Eqs. (18) or (43) representing either the background or radiance component of the errors, respectively. The matrix  $\mathbf{P}_{(f)}^a$  represents the background-error contribution, and  $\mathbf{P}_{(y)}^a$  the radiance-error contribution, to the analysis error covariance. Figure 3 shows the diagonal elements of these two matrices on a logarithmic scale, for the optimal (radiance analysis) case with  $\mathbf{K} = \mathbf{K}^{y_o}$  given by Eq. (46) and the suboptimal (interactive-retrieval analysis) case with  $\mathbf{K} = \mathbf{K}^{y_{so}}$  given by Eqs. (47) and (29).

Figure 3 shows that the interactive-retrieval analysis effectively assigns too much weight to the background and too little to the radiance data. The leading seven modes are well determined by the radiance data, so that the analysis errors for these modes are dominated by the radiance errors. The slightly increased weight given to the background, therefore, does not greatly affect the analysis in the leading modes. For the trailing seven modes, information from the background is largely dominant. In this regime, decreasing the weight given to the radiance data likewise does not significantly affect the analysis. For the middle modes (e.g. modes 8 and 9), the background and radiance errors are comparable. The suboptimal weighting in these modes may, therefore, produce some degradation in the analysis. As shown in Fig. 1, however, the overall degradation, as measured by analysis-error standard deviations, is small.

Figure 4 is similar to Fig. 3, but uses the Jacobian and error covariances for the HIRS instrument. The difference in weights in the cross-over modes (modes 2–4) appears to be more severe for HIRS than for AIRS. However, as shown in Fig. 1, the overall degradation in the suboptimal analysis is small in this case as well.

Table 1 shows the condition numbers of the innovation covariance matrices (i.e. the quantity to be inverted when solving the analysis equation) for radiance analysis and for optimal and suboptimal retrieval analysis for AIRS and HIRS. The numerical conditioning of the analysis equations is slightly better for suboptimal retrieval analysis

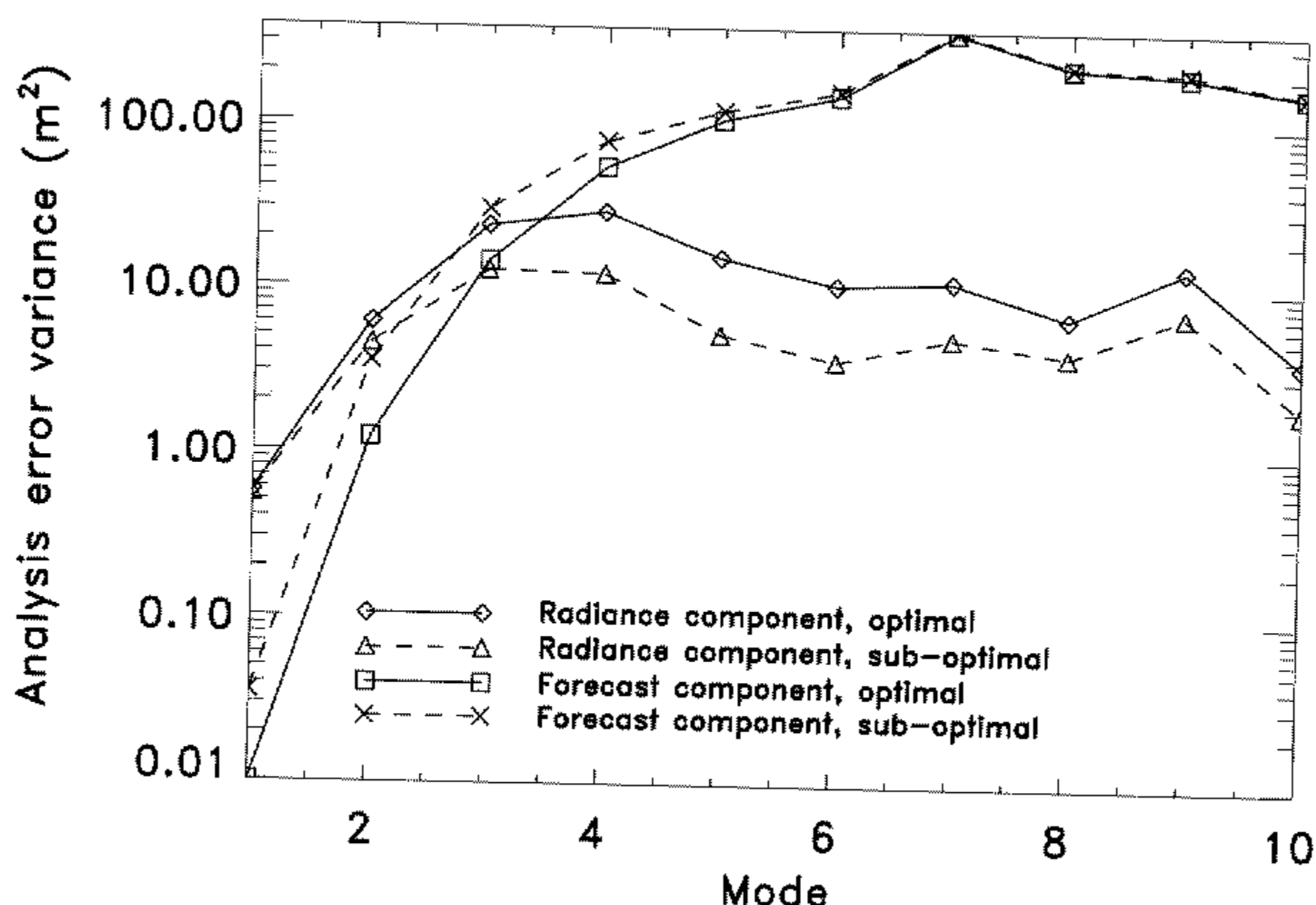


Figure 4. As Fig. 3, for simulated High-resolution InfraRed Sounder 2 data.

TABLE 1. CONDITION NUMBERS FOR THE INNOVATION COVARIANCE MATRIX

	AIRS	HIRS
Radiance assimilation	$3.25 \times 10^3$	$7.17 \times 10^2$
Retrieval assimilation, neglect $\mathbf{X}$ (sub-optimal)	$5.63 \times 10^2$	$6.39 \times 10^2$
Retrieval assimilation, account for $\mathbf{X}$ (optimal)	$7.59 \times 10^5$	$7.11 \times 10^8$

See text for further information.

than for radiance analysis. This implies that solving the analysis equations (in the PSAS context) will be somewhat more efficient for suboptimal retrieval analysis than for radiance analysis. The condition numbers for the innovation covariance associated with the optimal retrieval-analysis gain matrix Eq. (28) are very high, implying near singularity. This result is expected as explained in section 4 and by Eyre *et al.* (1993), and suggests that it will not be possible to assimilate retrievals from nadir-viewing instruments such as AIRS and HIRS with an optimal gain matrix.

(ii) *Using incorrect retrieval error covariances.* We now examine the effect of specifying incorrect retrieval error covariances in the analysis. This would occur in practice, for example, if the DAS employs a spatially invariant retrieval error-covariance model, even though actual retrieval errors are state-dependent. Equations (37) and (35) show how the interactive retrieval error covariances depend on the background and brightness-temperature error covariances, as well as on the Jacobian of the radiative-transfer model. The latter is state dependent due to the state dependence of the transmittances and the fact that brightness-temperature errors depend on scene brightness temperature. A colder scene brightness temperature corresponds to a higher noise-equivalent temperature. For example, the HIRS2 noise-equivalent temperatures for tropical and mid-latitude profiles differ by factors ranging from about 0.8 to 1.6, depending on the channel.

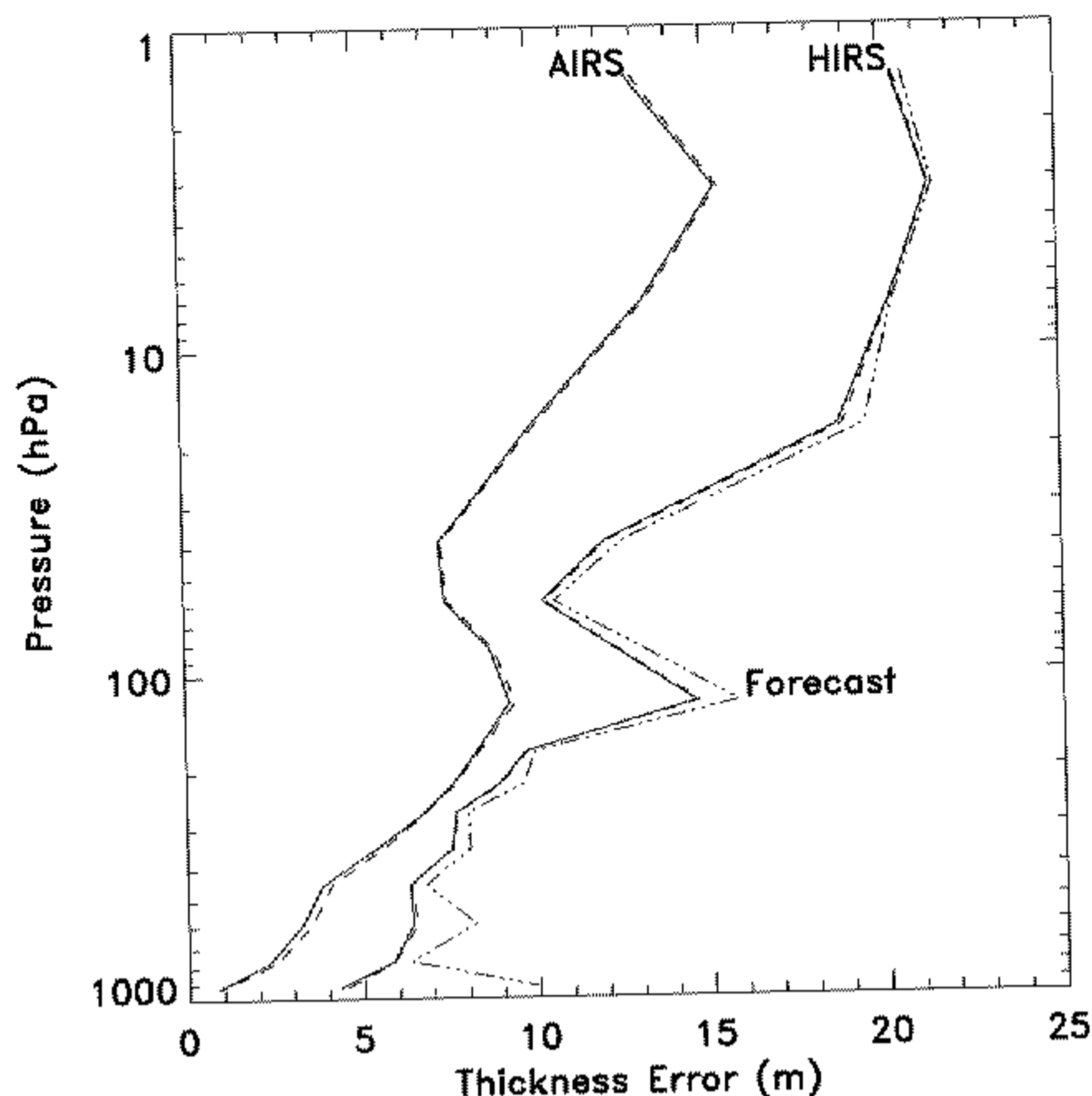


Figure 5. As Fig. 1, for a simulated tropical profile. Error covariances for the retrieval assimilation were incorrectly specified as for a mid-latitude profile.

For these experiments we specify the interactive retrieval error covariances using Eqs. (37) and (35) as before, but with Jacobians and brightness temperature error covariances computed for three different model-generated profiles, corresponding to low-, middle-, and high-latitude cases. These profiles are described in more detail in JS. We then simulate an analysis that used, for example, interactive retrievals in the tropics with a retrieval error covariance computed for the mid-latitude profile. The analysis is then suboptimal, not only because cross-covariances between retrieval and background errors are ignored, but also because the retrieval error covariances are mis-specified. We can still estimate the analysis error standard deviations for these cases, by means of Eq. (43) with the gain matrix defined by Eqs. (47) and (29).

Figure 5 shows the estimated thickness-error standard deviations for the tropical analysis with AIRS and HIRS, using incorrect error covariances based on the mid-latitude profile. The differences between the analysis errors for the optimal and sub-optimal cases are very small. We obtain similarly small differences for all other profile combinations. These results indicate that, for these 1D simulations, the analyses are not sensitive to small mis-specifications of the retrieval error covariance. In the previous section we showed that, in certain regimes, a mis-specification of the errors (e.g. neglecting retrieval/background cross-covariance) does not significantly harm the analysis. The results of this section imply that, in addition, a relatively small mis-specification of the retrieval error covariance also does not significantly degrade the suboptimal retrieval analysis. This result supports the use of spatially invariant retrieval error covariances for interactive clear-sky temperature retrieval analysis.

### (b) *Non-interactive retrieval analysis*

In order to simulate analysis errors that would be obtained with non-interactive retrieval analysis, we need to make assumptions about the accuracy of the prior-state

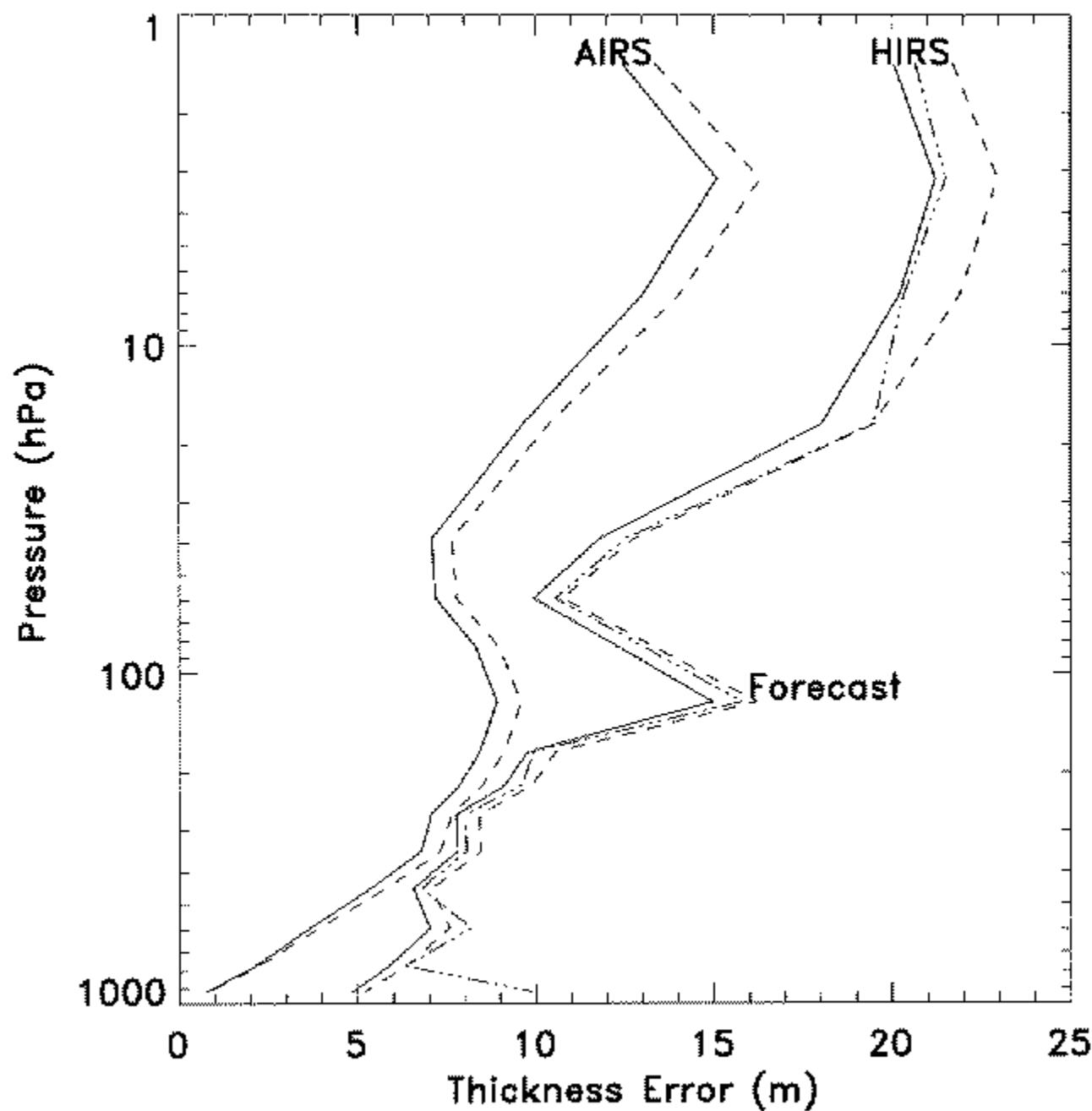


Figure 6. As Fig. 1, but for non-interactive retrieval assimilation, using  $\alpha = 1.5$ ,  $\gamma = 0.75$  for defining the error covariances. See text for further information.

estimate used for the retrieval, and about the cross-covariances between prior estimation and background errors; see Eq. (31). We are interested in the situation where a background from an older or different DAS or from some other source such as climatology is used as the prior information for the retrieval. In the next set of examples, we assume that the retrieval prior and analysis background error covariances take the same form (i.e. same vertical correlations). We then assume that the prior error variances ( $\sigma_p^2$ ) are larger than the analysis background variances ( $\sigma_f^2$ ) taking the form  $(\sigma_p^2) = \alpha^2 (\sigma_f^2)$ . To model the background–prior error cross-correlation, we multiply the fully correlated covariances by a factor  $\gamma$ , where  $\gamma \leq 1$ . Thus,  $\alpha = 1$ ,  $\gamma = 1$  corresponds to interactive retrievals. As  $\gamma \rightarrow 0$  the analysis errors may become smaller than those obtained with radiance analysis, because the prior-state estimate provides additional information. In reality, prior estimation errors and background errors are likely to be significantly correlated. As  $\gamma \rightarrow 1$  when  $\alpha > 1$ , the analysis should degrade. In this case the prior-state estimate, which contains little additional information with respect to the background, is assigned too much weight.

Figure 6 shows the estimated analysis errors for the case where the retrieval–prior error standard deviations are 50% larger than those of the background and the background–prior cross-covariance is about 0.75 ( $\alpha = 1.5$ ,  $\gamma = 0.75$ ). As before, solid curves correspond to (optimal) radiance analysis, and the dotted-dashed curve indicates the background error standard deviations. At some altitudes, the HIRS analysis errors exceed the background errors. Where the information content of the radiances is high, such as in the lower troposphere, the degradation with respect to the optimal analysis is small.

Figure 7 shows the same curves, but now with the prior-background cross-covariance reduced ( $\gamma = 0.25$ ). This corresponds to an increase in the amount of independent information contained in the prior-state estimate for the retrieval. As expected, the results

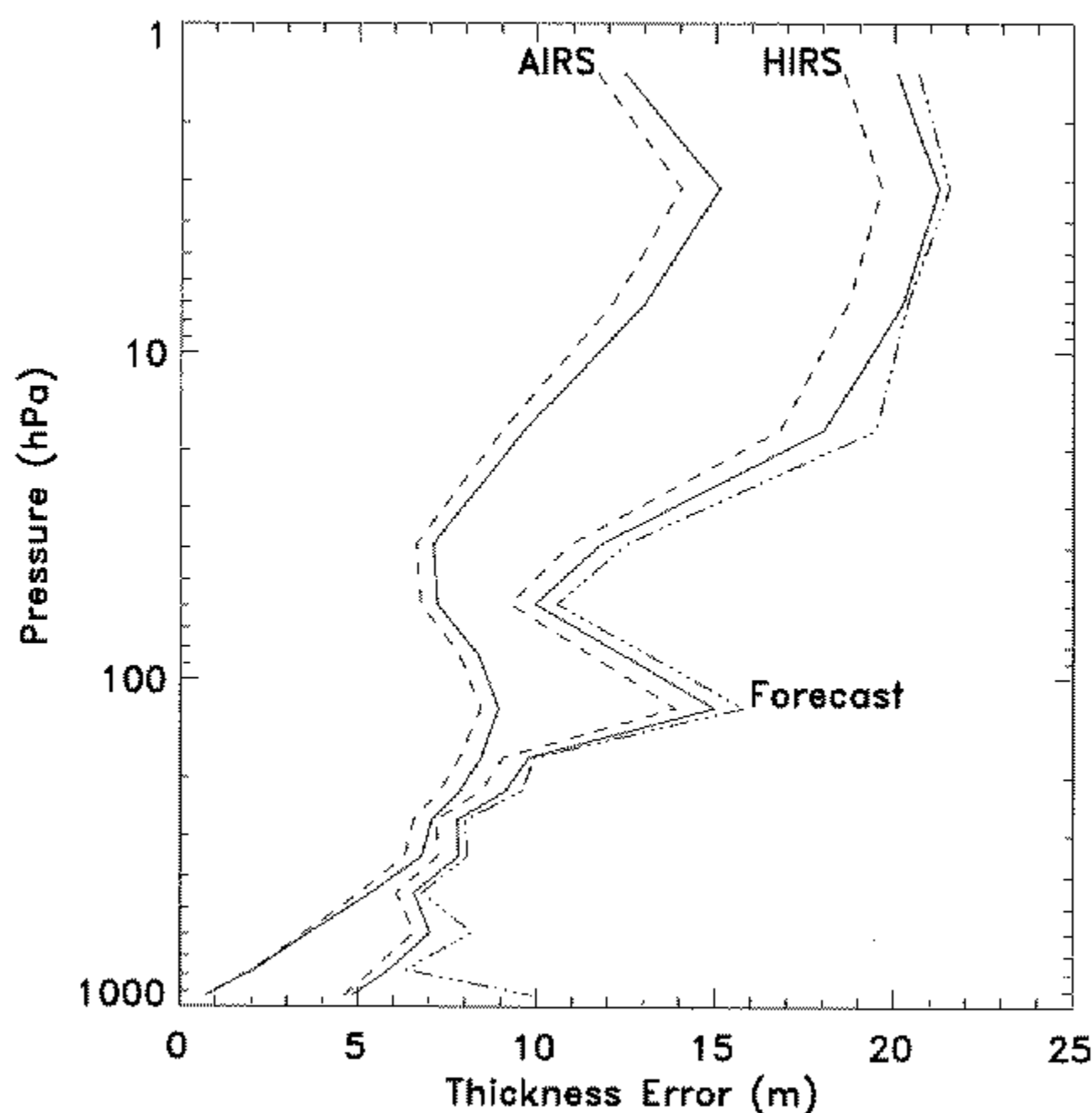


Figure 7. As Fig. 1, but for non-interactive retrieval assimilation, using  $\alpha = 1.5$ ,  $\gamma = 0.25$  for defining the error covariances. See text for further information.

improve as  $\gamma$  decreases; in fact, when  $\gamma = 0.25$  the analysis errors are smaller than those obtained with radiance analysis in almost every layer, even though  $\alpha > 1$ . When  $\alpha = 1.5$  and  $\gamma = 0.50$ , the result is nearly identical to optimal radiance analysis. The results of these experiments show that when analysing retrievals, the retrieval prior information and analysis background should have comparable errors. If this is the case, radiance and retrieval analyses should produce comparable results. If the retrieval prior errors are significantly larger than the analysis background errors, the resulting analysis can be significantly degraded.

## 6. CONCLUSIONS AND FUTURE WORK

We set out in this paper to compare different ways of utilizing satellite data, either by directly assimilating radiances in a variational framework or by first producing 1D retrievals and then assimilating the retrievals. Actual implementation of either method in an operational DAS involves numerous technical details, pertaining to quality control, systematic error correction, and covariance tuning. This begs the question whether the recent improvements in forecast skill obtained by centres that implemented direct radiance assimilation, is due to the change in methodology, or a result of various implementation details. In any case, computational and logistical arguments favour some form of retrieval assimilation for future high-volume data types, especially when using a PSAS-like analysis scheme. It is, therefore, important to learn as much as possible about the expected analysis errors for various suboptimal schemes, and to investigate whether any negative effects of retrieval assimilation are actually significant in view of the many uncertainties inherent in any data-assimilation method.

We presented a theoretical comparison of the analysis schemes used in analyses using radiances, interactive retrievals, and non-interactive retrievals. As has been pointed

out elsewhere, interactive retrieval analysis amounts to a suboptimal use of radiance data because cross-covariances between the retrieval and background errors are not accounted for in the analysis. We showed that, in fact, interactive retrieval analysis is linearly equivalent to radiance analysis with modified (hence suboptimal) analysis weights. We then showed that the resulting degradation of analysis accuracy is small for vertical modes that are determined mostly either by the radiances or by the background alone, but that the degradation can be significant for modes that are not well determined by either. Fortunately, this degradation does not appear to contribute much to the overall analysis errors.

These results were further clarified with a number of 1D numerical experiments, for which we simulated data from two different infrared sounders: AIRS and HIRS2. We found that the degradation of the analyses using interactive retrievals, rather than radiances, is insignificant in the context of these experiments. Moreover, the degradation was small even when we mis-specified retrieval error covariances. Whether this result holds true for more nonlinear problems, such as humidity analysis, remains to be seen. We also experimented with analysing non-interactive retrievals, varying the assumptions about the accuracy of the prior-state estimate used in the retrieval process and about the cross-covariances between the prior-estimation and background errors. We found that analysis of non-interactive retrievals can only be effective if the accuracy of the prior-state estimates used for producing the retrievals is at least comparable to that of the background used in the analysis system. If not, then the analyses may turn out significantly worse than in the case of either radiance or interactive retrieval analyses. In fact, analysis of retrievals produced with inferior prior-state estimates may actually result in analyses that are less accurate than the background itself.

Our conclusions are based on theoretical considerations combined with simple 1D simulations. There are obvious limitations to these experiments and the results may be somewhat optimistic. In the presence of other data types, such as radiosondes, that contain information on the higher-order vertical modes, retrieval assimilation could cause a significant over-weighting of the background. In addition, the analysis equations used here assume no bias in background and observation errors. Any bias present in the background would, again, tend to be over-weighted in retrieval assimilation. This may be particularly important when the retrieval contains prior information which is different from the assimilation background. There are some ways to address these concerns. For example, one might not assimilate retrievals when in the vicinity of radiosonde data. One could also apply a bias correction to the background field, as in Dee and da Silva (1998) and Dee and Todling (2000), to reduce the effects of background bias for interactive retrievals. Finally, we have considered here only temperature analysis, which is much more linear than humidity analysis. To address these concerns, we plan to do more sophisticated simulations with multiple data types in 3D to explore more fully the differences between radiance and suboptimal retrieval analyses. These simulations will include the effects of horizontal correlations in background errors and will address issues related to linearization and to representativeness of the observations on the scale of the estimation.

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